Exponential Monte Carlo Convergence of a Three-Dimensional Discrete Ordinates Solution

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INTRODUCTION

Recent work on obtaining exponential convergence for three-dimensional solutions to the spatially and angularly continuous monoenergetic transport equation with isotropic scattering using the reduced source method[1,2] was promising.[3] The method, however, used two separate estimates of the scalar flux, a Legendre expansion (in the spatial variables) and a quadrature of the angular flux. This introduced an inconsistency that may have lead to some convergence problems. To remove this inconsistency and provide a fairer test of the combined reduced source/Monte Carlo method, the method was applied to estimate the coefficients of a Legendre expansion of the solution of the discrete ordinates equations. In this case, no supplementary approximations were required.

THE REDUCED SOURCE METHOD

The monoenergetic neutral particle discrete ordinates equations in a homogeneous medium with isotropic scattering and no internal source can be written[4]

$$\hat{\mathbf{\Omega}}_m \cdot \nabla\psi_m(\mathbf{r}) + \Sigma_t \psi_m(\mathbf{r}) - \Sigma_s \sum_{m'=1}^{M} t_{m'} \psi_{m'}(\mathbf{r}) = 0 \quad , \quad m = 1, \ldots, M \quad , \tag{1}$$

with boundary condition

$$\left|\hat{\mathbf{\Omega}}_m \cdot \hat{\mathbf{n}}_s\right| \psi_m(\mathbf{r}_s) = S_m(\mathbf{r}_s) \quad , \quad \hat{\mathbf{\Omega}}_m \cdot \hat{\mathbf{n}}_s < 0 \quad . \tag{2}$$

Here, $\hat{\mathbf{\Omega}}_m$ and t_m represent the ordinates and weights of the discrete ordinates quadrature set.

Given some estimate $\tilde{\psi}_m(\mathbf{r})$ of the exact solution $\psi_m(\mathbf{r})$ of the discrete ordinates equations, the difference $\psi_m(\mathbf{r}) - \tilde{\psi}_m(\mathbf{r})$ is defined as the angular flux residual, $\Delta\psi_m(\mathbf{r})$. Using $\psi_m(\mathbf{r}) = \tilde{\psi}_m(\mathbf{r}) + \Delta\psi_m(\mathbf{r})$ in Eqs. (1) and (2) yields an equation for the angular flux residual:

$$\hat{\mathbf{\Omega}}_m \cdot \nabla\Delta\psi_m(\mathbf{r}) + \Sigma_t \Delta\psi_m(\mathbf{r}) - \Sigma_s \sum_{m'=1}^{M} t_{m'} \Delta\psi_{m'}(\mathbf{r}) = -\hat{\mathbf{\Omega}}_m \cdot \nabla\tilde{\psi}_m(\mathbf{r}) - \Sigma_t \tilde{\psi}_m(\mathbf{r}) + \Sigma_s \sum_{m'=1}^{M} t_{m'} \tilde{\psi}_{m'}(\mathbf{r}) \quad , \quad m = 1, \ldots, M \quad , \tag{3}$$

with boundary condition

$$\left|\hat{\mathbf{\Omega}}_m \cdot \hat{\mathbf{n}}_s\right| \Delta\psi_m(\mathbf{r}_s) = S_m(\mathbf{r}_s) - \left|\hat{\mathbf{\Omega}}_m \cdot \hat{\mathbf{n}}_s\right| \tilde{\psi}_m(\mathbf{r}_s) \quad , \quad \hat{\mathbf{\Omega}}_m \cdot \hat{\mathbf{n}}_s < 0 \quad . \tag{4}$$

In the reduced source method, Eq. (1) is solved for an initial estimate $\tilde{\psi}_m^0(\mathbf{r})$, which is then used on the right-hand sides of Eqs. (3) and (4) for the first order residual $\Delta\psi_m^1(\mathbf{r})$. Using the resulting estimate $\tilde{\psi}_m(\mathbf{r}) = \tilde{\psi}_m^0(\mathbf{r}) + \Delta\psi_m^1(\mathbf{r})$ on the right-hand sides of Eqs. (3) and (4) provides an equation for the second order residual $\Delta\psi_m^2(\mathbf{r})$ and a prescription for an iterative strategy. The angular flux estimate after *n* such iterations is $\tilde{\psi}_m(\mathbf{r}) = \tilde{\psi}_m^0(\mathbf{r}) + \sum_{n'=1}^{n} \Delta\psi_m^{n'}(\mathbf{r})$.

MONTE CARLO SCORING AND SAMPLING

In the present application of the method, the discrete ordinates fluxes $\psi_m(\mathbf{r})$ are expanded in Legendre polynomials as follows:

$$\psi_m(x,y,z) \approx \sum_{i=0}^{I} \sum_{j=0}^{J} \sum_{k=0}^{K} a_{m,ijk} P_i(\tfrac{2x}{X} - 1) P_j(\tfrac{2y}{Y} - 1) P_k(\tfrac{2z}{Z} - 1) \quad , \tag{5}$$

where the coefficients $a_{m,ijk}$ are defined as

$$a_{m,ijk} \equiv \frac{(2i+1)}{X} \frac{(2j+1)}{Y} \frac{(2k+1)}{Z} \int_0^X dx \int_0^Y dy \int_0^Z dz\, \psi_m(x,y,z) P_i(\tfrac{2x}{X} - 1) P_j(\tfrac{2y}{Y} - 1) P_k(\tfrac{2z}{Z} - 1) \quad . \tag{6}$$

Using a generalized track length estimator, a particle track of length *h* along ray *m* contributes a score

$$s(a_{m,ijk}) = \frac{(2i+1)}{X}\frac{(2j+1)}{Y}\frac{(2k+1)}{Z}\frac{w}{t_m}\int_0^h ds\, P_i(\tfrac{2x(s)}{X}-1)P_j(\tfrac{2y(s)}{Y}-1)P_k(\tfrac{2z(s)}{Z}-1) \qquad (7)$$

to the coefficient $a_{m,ijk}$ (w is the particle's weight). The angular quadrature weight t_m appears in the denominator because the track length estimator is used to estimate weighted integrals of the scalar flux rather than the angular flux.

The zero'th stage of the reduced source solution procedure, corresponding to an approximate solution of Eq. (1), is treated as a "conventional" (non-adaptive) Monte Carlo problem, except that the particles are constrained to travel along the pre-selected discrete ordinates. In subsequent (adaptive) stages, particles are started according to the residual sources $R_m^n(\mathbf{r})$, defined as the right-hand sides of Eqs. (3) and (4), which together describe a system with a volume source and a source on each surface. The solution to these equations is obtained by solving the problem for each source independently and adding those solutions.

Rather than sampling from the true (residual) source distribution $R_m^n(\mathbf{r})$, which may be positive or negative, particles are sampled uniformly in the appropriate phase space (uniformly in the volume and isotropically in angle for the volume source; uniformly on the surface and isotropically over the inward-directed half of the angle set for the surface sources). The particle weight w, which is the ratio of the true density to the sampled density, is $V\,R_m^n(\mathbf{r})$ for the volume source and $\frac{1}{2}A\,R_m^n(\mathbf{r}_s)$ for the surface sources. The particle weight can be negative.

As in deterministic discrete ordinates methods, the incoming fluxes must be properly normalized to preserve the physical source strength. In the present application, this is accomplished by using a properly normalized value for $S_m(\mathbf{r}_s)$ in Eq. (4).

RESULTS

The method was tested on a homogeneous three-dimensional slab of dimensions $1\ \text{cm} \times 10^6\ \text{cm} \times 10^6\ \text{cm}$ and material parameters $\Sigma_t = 1$ and $\Sigma_s = 0.5$. The external source of Eq. (2) was $S_m(\mathbf{r}_s) = S_m(0, y, z) = \mu_m$, $\mu_m > 0$. Figure 1 shows the results of the solution of the S_8 equations using a standard quadrature set, 560 000 particles per stage (except the zero'th, in which only 80 000 particles were used), and Legendre expansions of order 10 in each direction with no Legendre product terms in Eq. (5) [e.g., $a_{m,110}P_1(\frac{2x}{X}-1)P_1(\frac{2y}{Y}-1)$]. For this simple problem, Fig. 1 clearly shows exponential convergence of four different residuals and of two estimates of the known source. The difference between two Monte Carlo scalar fluxes (volume midpoint and volume average) and those estimated by THREEDANT (Ref. 5) using the same S_8 quadrature set are shown for verification. For this problem, convergence was achieved after 10 adaptive stages in 75.1 minutes.

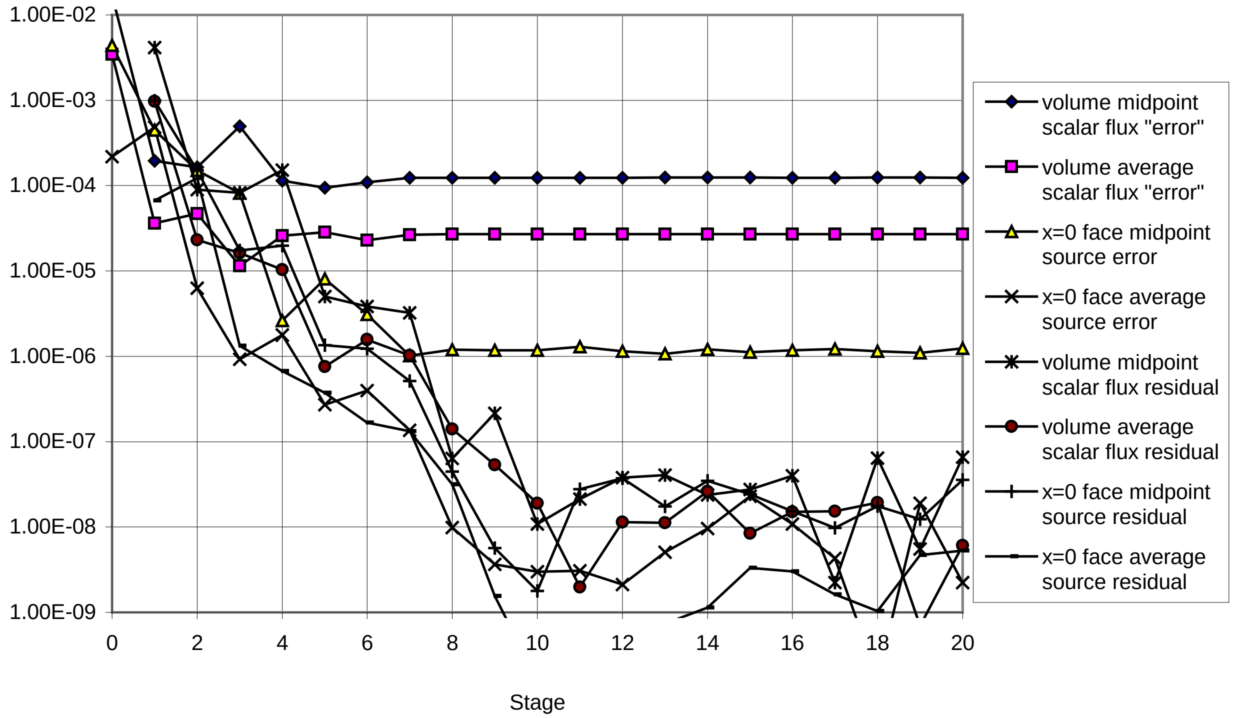

Figure 1. Exponential convergence of an S_8 solution in a three-dimensional slab. The method reproduces the exact incoming flux to about 10^{-6} (face midpoint) and below 10^{-7} (face average). The method reproduces the THREEDANT approximate solution for the scalar flux to about 10^{-4} (volume midpoint and volume average). Residuals for these four values converge exponentially to about 10^{-8}.

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